

# HIGH TEMPERATURE CONVERGENCE OF THE KMS BOUNDARY CONDITIONS: THE BOSE-HUBBARD MODEL ON A FINITE GRAPH

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**ABSTRACT.** The Kubo-Martin-Schwinger condition is a widely studied fundamental property in quantum statistical mechanics which characterises the thermal equilibrium states of quantum systems. In the seventies, G. Gallavotti and E. Verboven, proposed an analogue to the KMS condition for classical mechanical systems and highlighted its relationship with the Kirkwood-Salzburg equations and with the Gibbs equilibrium measures. In the present article, we prove that in a certain limiting regime of high temperature the classical KMS condition can be derived from the quantum condition in the simple case of the Bose-Hubbard dynamical system on a finite graph. The main ingredients of the proof are Golden-Thompson inequality, Bogoliubov inequality and semiclassical analysis.

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## 1. INTRODUCTION

A  $\mathscr{W}^*$ -dynamical system  $(\mathscr{A}, \tau_t)$  is a pair of a von Neumann algebra of observables  $\mathscr{A}$  and a one-parameter group of automorphisms  $\tau_t$  on  $\mathscr{A}$ . Consider for instance a finite dimensional Hilbert space  $\mathfrak{H}$  then  $\mathscr{A}$  can be chosen to be the set of all operators  $\mathcal{B}(\mathfrak{H})$  and  $\tau_t$  to be the automorphism group defined by

$$\tau_t(A) = e^{itH} A e^{-itH}$$

for any  $A \in \mathscr{A}$ . The operator  $H$  denotes the Hamiltonian of a given quantum system and the couple  $(\mathscr{A}, \tau_t)$  describes the dynamics. According to quantum statistical physics such system admits a unique thermal equilibrium state  $\omega_\beta$  at inverse temperature  $\beta$  given by,

$$\omega_\beta(A) = \frac{\text{tr}(e^{-\beta H} A)}{\text{tr}(e^{-\beta H})}. \quad (1.1)$$

In general, the simplicity of the above statement have to be nuanced. In fact, the characterisation of thermal equilibrium in statistical mechanics is a nontrivial question particularly for dynamical

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systems which have an infinite number of degrees of freedom, see [9, 26]. One of the important and most elegant characterisation of equilibrium states was noticed by R. Kubo, P.C. Martin and J. Schwinger in the late fifties. It is based in the following observations in finite dimension. In fact, one remarks by a simple computation that the Gibbs state  $\omega_\beta$  in (1.1) satisfies for all  $t \in \mathbb{R}$  and any  $A, B \in \mathcal{A}$  the identity,

$$\omega_\beta(A \tau_{t+i\beta}(B)) = \omega_\beta(\tau_t(B)A), \quad (1.2)$$

where  $\tau_{t+i\beta}(\cdot)$  denotes an analytic extension of the automorphism  $\tau_t$  to complex times given by

$$\tau_{t+i\beta}(B) = e^{(-\beta+it)H} B e^{(\beta-it)H}.$$

More remarkable, if one takes a state  $\omega$  that satisfies the same condition as (1.2) then  $\omega$  should be the Gibbs state  $\omega_\beta$  in (1.1). This indicates that the equation (1.2) singles out the thermal equilibrium states among all possible states of a quantum system. In the late sixties, R. Haag, N.M. Hugenholtz and M. Winnink suggested the identity (1.2) as a criterion for equilibrium states and they named it the KMS boundary condition after Kubo, Martin and Schwinger [19]. The subject of KMS states is bynow deeply studied specially from an algebraic standpoint. For instance, various characterisation related to correlation inequalities and to variational principles have been derived (see e.g. [13, 6, 9]). Other perspectives have also been explored related for instance to the Tomita-Takasaki theory and to the Heck algebra and number theory (see e.g. [11, 5, 7]).

In the seventies, G. Gallavotti and E. Verboven, suggested an analogue to the KMS boundary condition (1.2) which is suitable for classical mechanical systems and highlighted its relationship with the Kirkwood-Salzburg equations and with the Gibbs equilibrium measures, see [18]. The derivation of such condition is based in the following heuristic argument. Consider a state  $\omega_\hbar$  satisfying the KMS boundary condition

$$\omega_\hbar(BA) = \omega_\hbar(A \tau_{i\hbar\beta}(B)) \quad (1.3)$$

at inverse temperature  $\hbar\beta$ , where  $\hbar$  refers to the reduced Planck constant. This relation yields

$$\omega_\hbar\left(\frac{AB - BA}{i\hbar}\right) = \omega_\hbar\left(A \frac{\tau_{i\hbar\beta}(B) - B}{i\hbar}\right). \quad (1.4)$$

Assume for the moment that the space  $\mathfrak{H} = L^2(\mathbb{R}^d)$ , so one can consider that the Hamiltonian  $H$  and the observables  $A, B$  are given by  $\hbar$ -Weyl-quantized symbols (i.e.,  $H = \hbar^{W,\hbar}$ ,  $A = a^{W,\hbar}$  and  $B = b^{W,\hbar}$  for some smooth functions  $a$  and  $b$  defined over the phase-space  $\mathbb{R}^{2d}$ ). Then the semiclassical theory firstly tell us that

$$\frac{AB - BA}{i\hbar} \xrightarrow{\hbar \rightarrow 0} \{a, b\}, \quad \text{and} \quad \frac{\tau_{i\hbar\beta}(B) - B}{i\hbar} \xrightarrow{\hbar \rightarrow 0} \beta \{h, b\}, \quad (1.5)$$

where  $\{\cdot, \cdot\}$  is the Poisson bracket and  $h$  denotes the Hamiltonian of the corresponding classical system. Secondly, the quantum states  $\omega_\hbar$  (or at least a subsequence) converge in a weak sense to a semiclassical probability measure  $\mu$  over  $\mathbb{R}^{2d}$  when  $\hbar \rightarrow 0$ . Therefore, the expected classical KMS condition that should in principle characterise the statistical equilibrium for classical mechanical systems is formally given by

$$\mu(\{a, b\}) = \beta \mu(a \{h, b\}), \quad (1.6)$$

for any smooth functions  $a, b$  on the phase-space  $\mathbb{R}^{2d}$ . Here the notation  $\mu(f) = \int_{\mathbb{R}^{2d}} f(u) d\mu(u)$  is used. After the works [18, 1], M. Aizenman et al. showed in [2] that the condition (1.6) singles out thermal equilibrium states for infinite classical mechanical systems among all probability

measures. In particular, the only measure  $\mu$  satisfying (1.6) in our example is the Gibbs measure defined with respect to the Lebesgue measure by the density,

$$\mu_\beta = \frac{1}{z(\beta)} e^{-\beta h(u)}, \quad (1.7)$$

where  $z(\beta)$  is a normalisation constant. Note that the above Gibbs measure  $\mu_\beta$  can also be characterised as an equilibrium state by means of variational methods and maximum entropy properties or by correlation inequalities, see [9]. Nevertheless, in this note we focus only in the KMS boundary conditions for classical and quantum systems. In general, the derivation of the classical KMS boundary condition (1.6) from the quantum one is a non trivial and interesting question which depends on the considered dynamical system. In our opinion, the classical KMS condition is an elegant characterisation of statistical equilibrium which deserves more attention from PDE analysts. Although this condition has been studied in some subsequent works (see e.g. [17, 23, 25, 24, 10, 14]), it seems not largely known.

Our main purpose in this note, is to provide a rigorous and simple proof for the derivation of the classical KMS condition (1.6) as a consequence of the relation (1.2) and the classical limit,  $\hbar \rightarrow 0$ , for the Bose-Hubbard dynamical system on a finite graph. The system we consider is governed by a typical many-body quantum Hamiltonian which can be written in terms of creations annihilations operators and which is restricted to a finite volume. Our proof of convergence is based on the Golden-Thompson inequality, the Bogoliubov inequality and the semiclassical analysis in the Fock space. Since the classical phase-space of the system considered here is finite dimensional it is possible by change of representation to convert the problem to a semiclassical analysis in a  $L^2$  space. However, we avoid such a change as we lose most of the interesting insights and structures in our problem. In particular, we will rely on the analysis on the phase-space given in [3]. Our interest in the Bose-Hubbard system is motivated by the establishment of a strong link between classical and quantum KMS conditions so that it leads to the exchange of the thermodynamic and the classical limits for infinite dynamical systems and to the investigation of phase transitions. Also note that from a physical standpoint, the Bose-Hubbard model is a quite relevant model describing ultracold atoms in optical lattices with an observed phenomenon of superfluid-insulator transition. From a wider perspective, the question considered here is also related to the recent trend initiated by M. Lewin, P.T. Nam and N. Rougerie [21, 22] about the Gibbs measures for the nonlinear Schrödinger equations (see also [16] where these investigations were continued). In this respect, the KMS boundary conditions could provide an alternative proof for the convergence of Gibbs states. These questions will be considered elsewhere and here we will only focus on the Bose-Hubbard model on finite graph which is a much simpler model.

The article is organised as follows:

- In Section 2, the Bose-Hubbard Hamiltonian on a finite graph is introduced and its relationship with the discrete Laplacian is highlighted.
- Section 3, is dedicated to the description of the unique KMS state of the Bose-Hubbard dynamical system at inverse temperature  $\hbar\beta$  and to the extension of the dynamics to complex times.
- Section 4, contains our main contribution stated in Theorem 4.2. Indeed, we prove that the KMS states of the Bose-Hubbard system converge, up to subsequences, to semiclassical (Wigner) measures satisfying the classical KMS condition. The analysis is based on semiclassical methods in the Fock space developed in [3].
- Finally, in Section 5, we remark that any probability measure satisfying the classical KMS condition is indeed the Gibbs equilibrium measure for the Discret nonlinear Schrödinger equation. The proof of this fact is borrowed from the work [2].

## 2. QUANTUM HAMILTONIAN ON A FINITE GRAPH

*The discrete Laplacian:* Consider a finite graph  $G = (V, E)$  where  $V$  is the set of vertices and  $E$  is the set of edges. Assume furthermore that  $G$  is a simple undirected graph and let  $\deg(x)$  denotes the degree of each vertices  $x \in V$ . In the following, we denote the graph equivalently  $G$  or  $V$ . Consider the Hilbert space of all complex-valued functions on  $V$  denoted as  $\ell^2(G)$  and endowed with its natural scalar product and with the orthonormal basis  $(e_x)_{x \in V}$  such that

$$e_x(y) := \delta_{x,y}, \quad \forall x, y \in V.$$

Then the discrete Laplacian on the graph  $G$  is a non-positive bounded operator on  $\ell^2(G)$  given by,

$$(\Delta_G \psi)(x) := -\deg(x)\psi(x) + \sum_{y \in V, y \sim x} \psi(y),$$

with the above sum running over the nearest neighbours of  $x$  and  $\psi$  is any function in  $\ell^2(G)$ .

*The Bose-Hubbard Hamiltonian:* Consider the bosonic Fock space,

$$\mathfrak{F} = \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \otimes_s^n \ell^2(G),$$

where  $\otimes_s^n \ell^2(G)$  denotes the symmetric  $n$ -fold tensor product of  $\ell^2(G)$ . So, any  $\psi \in \otimes_s^n \ell^2(G)$  is a functions  $\psi : V^n \rightarrow \mathbb{C}$  invariant under any permutation of its variables. Introduce the usual creation and annihilation operators acting on the bosonic Fock space,

$$a_x = a(e_x) \quad \text{and} \quad a_x^* = a^*(e_x),$$

then the following canonical commutation relations are satisfied,

$$[a_x, a_y^*] = \delta_{x,y} \mathbf{1}_{\mathfrak{F}} \quad \text{and} \quad [a_x^*, a_y^*] = [a_x, a_y] = 0, \quad \forall x, y \in V.$$

**Definition 2.1** (Bose-Hubbard Hamiltonian). For  $\varepsilon \in (0, \bar{\varepsilon})$ ,  $\lambda > 0$  and  $\kappa < 0$ , define the  $\varepsilon$ -dependent Bose-Hubbard Hamiltonian on the bosonic Fock space  $\mathfrak{F}$  by

$$H_\varepsilon := \frac{\varepsilon}{2} \sum_{x, y \in V: y \sim x} (a_x^* - a_y^*)(a_x - a_y) + \frac{\varepsilon^2 \lambda}{2} \sum_{x \in V} a_x^* a_x^* a_x a_x - \varepsilon \kappa \sum_{x \in V} a_x^* a_x.$$

Here  $\lambda$  is the on-site interaction,  $\kappa$  is the chemical potential and  $\varepsilon$  is the semiclassical parameter.

*Remark 2.2.* The first term of the Hamiltonian  $H_\varepsilon$  is the kinetic part of the system and corresponds to the second quantization of the discrete Laplacian. Indeed, one can write

$$\frac{1}{2} \sum_{x, y \in V: y \sim x} (a_x^* - a_y^*)(a_x - a_y) = \sum_{x \in V} \deg(x) a_x^* a_x - \sum_{x, y \in V, y \sim x} a_x^* a_y = d\Gamma(-\Delta_G),$$

where  $d\Gamma(\cdot)$  is the second quantization operator defined on the bosonic Fock space by

$$d\Gamma(A)_{|\otimes_s^n \ell^2(G)} = \sum_{j=1}^n 1 \otimes \cdots \otimes A^{(j)} \otimes \cdots \otimes 1, \quad (2.1)$$

for any given operator  $A \in \mathcal{B}(\ell^2(G))$  and where  $A^{(j)}$  means that  $A$  acts only in the  $j$ -th component.

The following rescaled *number operator* will be often used,

$$N_\varepsilon := \varepsilon d\Gamma(1_{\ell^2(G)}) = \varepsilon \sum_{x \in V} a_x^* a_x. \quad (2.2)$$

Therefore, one can rewrite the Bose-Hubbard Hamiltonian as follows

$$H^\varepsilon = \varepsilon \, \mathrm{d}\Gamma\big(-\Delta_G - \kappa 1_{\ell^2(G)}\big) + \varepsilon^2 \frac{\lambda}{2} I_G,$$

with the interaction denoted as

$$I_G := \sum_{x \in V} a_x^* a_x^* a_x a_x.$$

Since the discrete Laplacian  $\Delta_G$  is self-adjoint, it is easy to check that  $H_\varepsilon$  defines an (unbounded) self-adjoint operator on the Fock space  $\mathfrak{F}$  over its natural domain (for more details see e.g. [4, Appendix A]). Remark that the operator  $-\Delta_G - \kappa 1_{\ell^2(G)}$  is positive since the chemical potential  $\kappa$  is negative.

### 3. QUANTUM KMS CONDITION

The Bose-Hubbard Hamiltonian defines a  $\mathscr{W}^*$ -dynamical system  $(\mathfrak{M}, \alpha_t)$  where  $\mathfrak{M}$  is the von Neumann algebra of all bounded operators  $\mathcal{B}(\mathfrak{F})$  on the Fock space and  $\alpha_t$  is the one parameter group of automorphisms defined by

$$\alpha_t(A) = e^{i\frac{t}{\varepsilon} H_\varepsilon} A e^{-i\frac{t}{\varepsilon} H_\varepsilon},$$

for any  $A \in \mathfrak{M}$ . The above group of automorphisms  $\alpha_t$  admits a generator  $S : \mathfrak{M} \rightarrow \mathfrak{M}$  with a domain

$$\mathcal{D}(S) = \{A \in \mathfrak{M}, [H_\varepsilon, A] \in \mathfrak{M}\},$$

and satisfies for any  $A \in \mathcal{D}(S)$ ,

$$S(A) = \lim_{t \rightarrow 0} \frac{\alpha_t(A) - A}{t} = \frac{i}{\varepsilon} [H_\varepsilon, A].$$

The latter convergence is with respect to the  $\sigma$ -weak topology on  $\mathfrak{M}$ . Remark also that the dynamics  $\alpha_t$  depend on the semiclassical parameter  $\varepsilon$ .

Next, we point out that the dynamical system  $(\mathfrak{M}, \alpha_t)$  admits a unique KMS state at inverse temperature  $\varepsilon\beta$ . Here  $\beta > 0$  is a fixed,  $\varepsilon$ -independent, effective inverse temperature.

**Lemma 3.1** (Partition function).

*Since the chemical potential  $\kappa$  is negative then*

$$\mathrm{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon}) < \infty.$$

*Proof.* It is a consequence of [9, Proposition 5.2.27] and the Golden-Thompson inequality. The latter, see [15], says that for any Hermitian matrices  $A$  and  $B$  one has,

$$\mathrm{tr}(e^{A+B}) \leq \mathrm{tr}(e^A e^B). \quad (3.1)$$

□

**Definition 3.2** (Gibbs state).

The Gibbs equilibrium state of the Bose-Hubbard system on a finite graph is well defined, according to Lemma 3.2, and it is given by

$$\omega_\varepsilon(A) = \frac{\mathrm{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon} A)}{\mathrm{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon})}. \quad (3.2)$$

For the sake of completeness, we recall some useful details concerning the KMS states. One says that  $A \in \mathfrak{M}$  is an *entire analytic element* of  $\alpha_t$  if there exists a function  $f : \mathbb{C} \rightarrow \mathfrak{M}$  such that  $f(t) = \alpha_t(A)$  for all  $t \in \mathbb{R}$  and such that for any trace-class operator  $\rho \in \mathfrak{M}$  the function  $z \in \mathbb{C} \rightarrow \mathrm{tr}(\rho f(z))$  is analytic. Let  $\mathfrak{M}_\alpha$  denotes the set of entire analytic elements for  $\alpha$ , then it is known that  $\mathfrak{M}_\alpha$  is dense in  $\mathfrak{M}$  with respect to the  $\sigma$ -weak topology. For more details on analytic

elements, see [8, section 2.5.3]. In particular, by [8, Definition 2.5.20], an element  $A \in \mathfrak{M}$  is entire analytic if and only if  $A \in \mathcal{D}(S^n)$  for all  $n \in \mathbb{N}$  and for any  $t > 0$  the series below are absolutely convergent,

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} \|S^n(A)\| < \infty. \quad (3.3)$$

Remark that on the set of entire analytic elements  $\mathfrak{M}_\alpha$ , the dynamics  $\alpha_t$  can be extends to complex times. Indeed,  $\alpha_z(A)$  is well defined, for any  $A \in \mathfrak{M}_\alpha$ , by the following absolutely convergent series,

$$\alpha_z(A) = \sum_{n=0}^{\infty} \frac{z^n}{n!} S^n(A), \quad \forall z \in \mathbb{C}.$$

We say that a state  $\omega$  is a  $(\alpha_t, \varepsilon\beta)$ -KMS state if and only if  $\omega$  is normal and for any  $A, B \in \mathfrak{M}_\alpha$ ,

$$\omega(A \alpha_{i\varepsilon\beta}(B)) = \omega(BA). \quad (3.4)$$

Remark that the above identity is known to be equivalent to the condition stated in the introduction (1.2). In particular, the KMS states are stationary states with respect to the dynamics.

**Proposition 3.3.** *The Gibbs state  $\omega_\varepsilon$  defined by (3.2) is the unique KMS state of the  $\mathscr{W}^*$ -dynamical system  $(\mathfrak{M}, \alpha_t)$  at the inverse temperature  $\varepsilon\beta$ .*

*Proof.* For  $A, B \in \mathfrak{M}_\alpha$ , one checks

$$\alpha_{i\varepsilon\beta}(B) = e^{-\beta H_\varepsilon} B e^{\beta H_\varepsilon}.$$

The formula (3.2) for the Gibbs state, gives

$$\omega_\varepsilon(A \alpha_{i\varepsilon\beta}(B)) = \frac{1}{\text{tr}_{\mathfrak{F}}(e^{-\beta H_\varepsilon})} \text{tr}_{\mathfrak{F}}(A e^{-\beta H_\varepsilon} B) = \omega_\varepsilon(BA).$$

Reciprocally, let  $\omega$  be a  $(\alpha_t, \varepsilon\beta)$ -KMS state. In particular, there exists a density matrix  $\rho$  such that  $\text{tr}_{\mathfrak{F}}(\rho) = 1$  and

$$\omega(A) = \text{tr}_{\mathfrak{F}}(\rho A), \quad \forall A \in \mathfrak{M}.$$

Using the KMS condition (3.4) and the cyclicity of the trace, one proves for any  $A \in \mathfrak{M}$ ,

$$\text{tr}(\rho B A) = \text{tr}(e^{-\beta H_\varepsilon} B e^{\beta H_\varepsilon} \rho A).$$

In particular, for any  $B \in \mathfrak{M}_\alpha$ ,

$$\rho B = e^{-\beta H_\varepsilon} B e^{\beta H_\varepsilon} \rho. \quad (3.5)$$

Hence, one remarks that  $\rho$  commutes with any spectral projection of  $H_\varepsilon$  by taking for instance  $B = 1_D(H_\varepsilon)$  in the equation (3.5). Therefore, one concludes that

$$e^{\beta H_\varepsilon} \rho B_{|1_D(H_\varepsilon)\mathfrak{F}} = B e^{\beta H_\varepsilon} \rho_{|1_D(H_\varepsilon)\mathfrak{F}},$$

for any bounded Borel subset  $D$  of  $\mathbb{R}$  and any bounded operator  $B$  satisfying  $B = 1_D(H_\varepsilon)B = B1_D(H_\varepsilon)$ . So, the operator  $e^{\beta H_\varepsilon} \rho$  commutes with any bounded operator over the subspaces  $1_D(H_\varepsilon)\mathfrak{F}$ . This implies that

$$\rho = c e^{-\beta H_\varepsilon},$$

and then one concludes with the fact that  $\text{tr}(\rho) = 1$ .  $\square$

## 4. CONVERGENCE

In this section, we prove that the KMS condition (3.4) converges, in the classical limit, towards the classical KMS condition. It is enough to prove such convergence for some specific observables  $A, B \in \mathfrak{M}$ . In fact, consider for  $f, g \in \ell^2(G)$ ,

$$A = W(f), \quad \text{and} \quad B = W(g), \quad (4.1)$$

where  $W(\cdot)$  denotes the Weyl operator defined by,

$$W(f) = e^{i\sqrt{\varepsilon} \Phi(f)}, \quad \text{with} \quad \Phi(f) = \frac{a^*(f) + a(f)}{\sqrt{2}}. \quad (4.2)$$

Let  $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$  such that  $0 \leq \chi \leq 1$ ,  $\chi \equiv 1$  if  $|x| \leq 1/2$  and  $\chi \equiv 0$  if  $|x| \geq 1$ . Define, for  $n \in \mathbb{N}$ , the cut-off functions  $\chi_n$  as

$$\chi_n(\cdot) = \chi\left(\frac{\cdot}{n}\right).$$

Then, we are going to consider only the following smoothed observables,

$$A_n := \chi_n(N_\varepsilon) A \chi_n(N_\varepsilon), \quad \text{and} \quad B_n := \chi_n(N_\varepsilon) B \chi_n(N_\varepsilon). \quad (4.3)$$

**Lemma 4.1.** *For all  $\varepsilon > 0$  and  $n \in \mathbb{N}$ , the elements  $A_n$  and  $B_n$  given by (4.3) are entire analytic for the dynamics  $\alpha_t$ .*

*Proof.* By functional calculus, remark that  $1_{[0,n]}(N_\varepsilon) \chi_n(N_\varepsilon) = \chi_n(N_\varepsilon)$ . Moreover, the number operator  $N_\varepsilon$  and the Hamiltonian  $H_\varepsilon$  commute in the strong sense. So, the generator  $S$  of the dynamics  $\alpha_t$  satisfies for  $k \in \mathbb{N}$ ,

$$\begin{aligned} S^k(A_n) &= \left(\frac{i}{\varepsilon}\right)^k [H_\varepsilon, \dots [H_\varepsilon, A_n] \dots], \\ &= \left(\frac{i}{\varepsilon}\right)^k [\tilde{H}_\varepsilon, \dots [\tilde{H}_\varepsilon, A_n] \dots], \end{aligned}$$

with  $\tilde{H}_\varepsilon = 1_{[0,n]}(N_\varepsilon) H_\varepsilon$  a bounded operator. Hence, the estimate (3.3) is satisfied and so  $A_n$  is a entire analytic element.  $\square$

Recall that the  $(\alpha_t, \varepsilon\beta)$ -KMS state  $\omega_\varepsilon$  satisfies in particular the condition,

$$\omega_\varepsilon(A_n \alpha_{i\varepsilon\beta}(B_m)) = \omega_\varepsilon(B_m A_n).$$

A simple computation then leads to the main identity,

$$\omega_\varepsilon\left(A_n \frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon}\right) = \omega_\varepsilon\left(\frac{[B_m, A_n]}{i\varepsilon}\right). \quad (4.4)$$

Our aim is to take the classical limit  $\varepsilon \rightarrow 0$  in the above relation and to prove the convergence for the left and right hand sides so that we obtain the classical KMS boundary conditions. In order to take such limit, one needs to use the semiclassical (Wigner) measures of  $\{\omega_\varepsilon\}_{\varepsilon \in (0, \bar{\varepsilon})}$ . Recall that  $\mu$  a Borel probability measure on the phase-space  $\ell^2(G)$  is a Wigner measure of  $\{\omega_\varepsilon\}_{\varepsilon \in (0, \bar{\varepsilon})}$  if there exists a subsequence  $(\varepsilon_k)_{k \in \mathbb{N}}$  such that  $\lim_{k \rightarrow \infty} \varepsilon_k = 0$  and for any  $f \in \ell^2(G)$ ,

$$\lim_{k \rightarrow \infty} \omega_{\varepsilon_k}(W(f)) = \int_{\ell^2(G)} e^{i\sqrt{2}\Re\langle f, u \rangle} d\mu. \quad (4.5)$$

Note that the Weyl operator depends here on the parameter  $\varepsilon_k$  instead of  $\varepsilon$  as in (4.2). According to [3, Thm. 6.2] and Lemma A.3, the family of KMS states  $\{\omega_\varepsilon\}_{\varepsilon \in (0, \bar{\varepsilon})}$  admits a non-void set of Wigner probability measures. Later on, we will prove that this set of measures reduces to a singleton given by the Gibbs equilibrium measure. But for the moment, we will use subsequences as in the definition (4.5).

The classical Hamiltonian system related to the Bose-Hubbard model is given by the *Discrete Nonlinear Schrödinger* equation, see [20]. Its energy functional (or Hamiltonian) is given by

$$h(u) = -\langle u, \Delta_G u \rangle - \kappa \|u\|^2 + \frac{\lambda}{2} \sum_{j \in V} |u(j)|^4. \quad (4.6)$$

Note that  $\ell^2(G)$  is a complex Hilbert space and so in our framework the Poisson structure is defined as follows. For  $F, G$  smooth functions on  $\ell^2(G)$ , the Poisson bracket is given by

$$\{F, G\} := \frac{1}{i} (\partial_u F \cdot \partial_{\bar{u}} G - \partial_{\bar{u}} F \cdot \partial_u G). \quad (4.7)$$

Here  $\partial_u$  and  $\partial_{\bar{u}}$  are the standard differentiation with respect to  $u$  or  $\bar{u}$ .

Our main result is stated below.

**Theorem 4.2** (Classical KMS condition). *Let  $\omega_\varepsilon$  be the KMS state of the Bose-Hubbard  $\mathcal{W}^*$ -dynamical system  $(\mathcal{A}, \alpha_t)$  at inverse temperature  $\varepsilon\beta$ . Then any semiclassical (Wigner) measure of  $\omega_\varepsilon$  satisfies the classical KMS condition, i.e., for any  $F, G$  smooth functions on  $\ell^2(G)$ ,*

$$\beta \mu(\{h, G\} F) = \mu(\{F, G\}), \quad (4.8)$$

where the classical Hamiltonian  $h$  is given by (4.6) and  $\{\cdot, \cdot\}$  denotes the Poisson bracket recalled in (4.7).

In order to prove Theorem 4.2, one needs some preliminary steps.

**Proposition 4.3.** *Let  $(\varepsilon_k)_{k \in \mathbb{N}}$  be a subsequence such that  $\lim_{k \rightarrow \infty} \varepsilon_k = 0$ . Assume that the family of KMS states  $\{\omega_{\varepsilon_k}\}_{k \in \mathbb{N}}$  admits a unique Wigner measure  $\mu$ . Then for all  $n, m$  integers such that  $m \geq 2n$ ,*

$$\lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( \frac{[B_m, A_n]}{i\varepsilon_k} \right) = \int_{\ell^2(G)} \chi_n^2(\langle u, u \rangle) \{e^{\sqrt{2}i\Re\langle g, u \rangle}; e^{\sqrt{2}i\Re\langle f, u \rangle}\} d\mu \quad (4.9)$$

$$+ \int_{\ell^2(G)} \chi_n(\langle u, u \rangle) \{e^{\sqrt{2}i\Re\langle g, u \rangle}; \chi_n(\langle u, u \rangle)\} e^{\sqrt{2}i\Re\langle f, u \rangle} d\mu \quad (4.10)$$

$$+ \int_{\ell^2(G)} \chi_n(\langle u, u \rangle) \{\chi_n(\langle u, u \rangle); e^{\sqrt{2}i\Re\langle f, u \rangle}\} e^{\sqrt{2}i\Re\langle g, u \rangle} d\mu. \quad (4.11)$$

*Proof.* For simplicity, we denote  $\varepsilon$  instead of  $\varepsilon_k$  and  $\chi_m$  instead of  $\chi_m(N_\varepsilon)$ . Using the cyclicity of the trace and the fact that  $\chi_n \chi_m = \chi_n$ , one remarks that

$$\omega_\varepsilon([B_m, A_n]) = \omega_\varepsilon(\chi_n(B\chi_n A - A\chi_n B)).$$

A simple computation yields,

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \frac{[B_m, A_n]}{i\varepsilon} \right) &= \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n^2 \frac{[B, A]}{i\varepsilon} \right) \\ &+ \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n \frac{[B, \chi_n]}{i\varepsilon} A \right) \\ &+ \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n \frac{[\chi_n, A]}{i\varepsilon} B \right). \end{aligned} \quad (4.12)$$

The Weyl commutation relations give,

$$\frac{[B, A]}{i\varepsilon} = W(f + g) (\Im \langle f, g \rangle + O(\varepsilon)).$$



So, using Lemma B.1,

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n^2 \frac{[B, A]}{i\varepsilon} \right) &= \Im \langle f, g \rangle \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon (\chi_n^2 W(f+g)) \\ &= \Im \langle f, g \rangle \int_{\ell^2(G)} \chi_n^2(\langle u, u \rangle) e^{\sqrt{2}i\Re \langle f+g, u \rangle} d\mu. \end{aligned}$$

Checking the Poisson bracket,

$$\{e^{\sqrt{2}i\Re \langle g, u \rangle}; e^{\sqrt{2}i\Re \langle f, u \rangle}\} = \Im \langle f, g \rangle e^{\sqrt{2}i\Re \langle f+g, u \rangle},$$

one obtains the right hand side of (4.9). Consider now the second term in (4.12). One can write

$$[W(g), \chi_n] = \int_{\mathbb{R}} \hat{\chi}_n(s) [W(g), e^{isN_\varepsilon}] \frac{ds}{\sqrt{2\pi}},$$

where  $\hat{\chi}_n$  denotes the Fourier transform of the function  $\chi_n(\cdot)$ . Using standard computations in the Fock space and Taylor expansion,

$$\begin{aligned} [W(g), e^{isN_\varepsilon}] &= e^{isN_\varepsilon} (e^{-isN_\varepsilon} W(g) e^{isN_\varepsilon} - W(g)) \\ &= ie^{isN_\varepsilon} \int_0^s e^{-irN_\varepsilon} [W(g), N_\varepsilon] e^{irN_\varepsilon} dr \\ &= -e^{isN_\varepsilon} \int_0^s e^{-irN_\varepsilon} W(g) \left( \varepsilon \Phi(ig) + \frac{\varepsilon^2}{2} \|g\|^2 \right) e^{irN_\varepsilon} dr. \end{aligned}$$

Hence, using the cyclicity of the trace

$$\lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n \frac{[B, \chi_n]}{i\varepsilon} A \right) = - \int_{\mathbb{R}} s \hat{\chi}_n(s) \lim_{\varepsilon \rightarrow 0} \omega_\varepsilon (\chi_n e^{isN_\varepsilon} W(g) \Phi(ig) W(f)) \frac{ds}{\sqrt{2\pi}}. \quad (4.13)$$

Knowing, by Lemma B.1, that the Wigner measure of the sequence  $\{W(f)\rho_\varepsilon \chi_n(N_\varepsilon) e^{isN_\varepsilon} W(g)\}$  is given by

$$\{\mu \chi_n(\langle u, u \rangle) e^{is\|u\|^2} e^{\sqrt{2}i\Re \langle g+f, u \rangle}\},$$

then one obtains using [3, Thm. 6.13],

$$\lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n \frac{[B, \chi_n]}{i\varepsilon} A \right) = -\sqrt{2} \int_{\mathbb{R}} s \hat{\chi}_n(s) \int_{\ell^2(G)} \chi_n(\langle u, u \rangle) e^{is\|u\|^2} \Re \langle u, ig \rangle e^{\sqrt{2}i\Re \langle g+f, u \rangle} d\mu \frac{ds}{\sqrt{2\pi}}.$$

Integrating back with respect to the variable  $s$ ,

$$\lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( \chi_n \frac{[B, \chi_n]}{i\varepsilon} A \right) = \sqrt{2}i \int_{\ell^2(G)} \chi'_n(\|u\|^2) \chi_n(\|u\|^2) \Im \langle g, u \rangle e^{\sqrt{2}i\Re \langle g+f, u \rangle} d\mu.$$

Then checking the Poisson bracket

$$\{e^{\sqrt{2}i\Re \langle g, u \rangle}; \chi_n(\langle u, u \rangle)\} = \sqrt{2}i \chi'_n(\|u\|^2) \Im \langle g, u \rangle e^{\sqrt{2}i\Re \langle g, u \rangle},$$

yields the right hand side of (4.10). The third term in the right side of (4.12) is similar to the above one.  $\square$

The next step is to prove the convergence of the left hand side of (4.4).

**Lemma 4.4.**

$$\lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( A_n \frac{\alpha_{i\varepsilon_k \beta}(B_m) - B_m}{i\varepsilon_k} \right) = \beta \lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( A_n \frac{[B_m, H_{\varepsilon_k}]}{i\varepsilon_k} \right). \quad (4.14)$$

*Proof.* For simplicity, we use  $\varepsilon$  instead of  $\varepsilon_k$ . According to Lemma 4.1,  $B_m$  is a entire analytic element for the dynamics  $\alpha_t$ . Hence, by Taylor expansion,

$$\omega_\varepsilon \left( A_n \frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon} \right) = \beta \int_0^1 \omega_\varepsilon \left( A_n \frac{[\alpha_{is\varepsilon\beta}(B_m), H_\varepsilon]}{i\varepsilon} \right) ds.$$

Using the cyclicity of the trace and the fact that  $A_n, B_m$  are entire analytic elements,

$$\omega_\varepsilon \left( A_n \frac{[\alpha_{is\varepsilon\beta}(B_m), H_\varepsilon]}{i\varepsilon} \right) = \omega_\varepsilon \left( e^{s\beta H_\varepsilon} A_n e^{-s\beta H_\varepsilon} \frac{[B_m, H_\varepsilon]}{i\varepsilon} \right).$$

A second Taylor expansion yields,

$$\begin{aligned} \omega_\varepsilon \left( A_n \frac{[\alpha_{is\varepsilon\beta}(B_m), H_\varepsilon]}{i\varepsilon} \right) &= \omega_\varepsilon \left( A_n \frac{[B_m, H_\varepsilon]}{i\varepsilon} \right) \\ &\quad + \beta \int_0^s \omega_\varepsilon \left( e^{r\beta H_\varepsilon} [H_\varepsilon, A_n] e^{-r\beta H_\varepsilon} \frac{[B_m, H_\varepsilon]}{i\varepsilon} \right) dr. \end{aligned}$$

So, the equality (4.14) is proved since

$$\lim_{\varepsilon \rightarrow 0} \int_0^1 ds \int_0^s dr \omega_\varepsilon \left( [H_\varepsilon, \alpha_{-is\varepsilon\beta}(A_n)] \frac{[B_m, H_\varepsilon]}{i\varepsilon} \right) = 0,$$

thanks to the Lemma B.2 in the Appendix.  $\square$

**Proposition 4.5.** *Let  $(\varepsilon_k)_{k \in \mathbb{N}}$  be a subsequence such that  $\lim_{k \rightarrow \infty} \varepsilon_k = 0$ . Assume that the family of KMS states  $\{\omega_{\varepsilon_k}\}_{k \in \mathbb{N}}$  admits a unique Wigner measure  $\mu$ . Then for all  $n, m$  integers such that  $m \geq 2n$ ,*

$$\lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( A_n \frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon} \right) = \beta \int_{\ell^2(G)} \chi_n^2(\langle u, u \rangle) \{e^{\sqrt{2}i\Re\langle g, u \rangle}; h(u)\} e^{\sqrt{2}i\Re\langle f, u \rangle} d\mu. \quad (4.15)$$

*Proof.* The previous Lemma 4.4 allowed to get rid of the dynamics at complex times. So, it is enough to show the limit,

$$\lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( A_n \frac{[B_m, H_{\varepsilon_k}]}{i\varepsilon_k} \right) = \int_{\ell^2(G)} \chi_n^2(\langle u, u \rangle) \{e^{\sqrt{2}i\Re\langle g, u \rangle}; h(u)\} e^{\sqrt{2}i\Re\langle f, u \rangle} d\mu.$$

For simplicity, we denote  $\varepsilon$  instead of  $\varepsilon_k$  and  $\chi_m$  instead of  $\chi_m(N_\varepsilon)$ . Since  $m \geq 2n$  then  $\chi_n \chi_m = \chi_n$  and one notices that

$$\chi_n A \chi_n [\chi_m B \chi_m, H_\varepsilon] = \chi_n A \chi_n [B, H_\varepsilon] \chi_m = \chi_n A \chi_n [W(g), H_\varepsilon] \chi_m.$$

Standard computations on the Fock space yield, (see e.g. [3, Proposition 2.10]),

$$\begin{aligned} \frac{i}{\varepsilon} [B, H_\varepsilon] &= \frac{i}{\varepsilon} (W(g) H_\varepsilon W(g)^* - H) W(g) \\ &= \frac{i}{\varepsilon} \left( h(\cdot - \frac{i\varepsilon}{\sqrt{2}} g) - h(u) \right)^{Wick} W(g) \\ &= \left( \underbrace{\{\sqrt{2}\Re\langle g, u \rangle, h(u)\}}_{C^{Wick}} + R(\varepsilon)^{Wick} \right) W(g). \end{aligned}$$

The subscript *Wick* refers to the Wick quantization, see [3, section 2]. The remainder  $R(\varepsilon)^{Wick}$  can be explicitly computed and satisfies the uniform estimate

$$\|\chi_n(N_\varepsilon) R(\varepsilon)^{Wick}\| \leq c \varepsilon,$$

which can be easily proved using [3, Lemma 2.5]. Therefore, by using Lemma B.2 one shows

$$\begin{aligned} \lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( A_n \frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon} \right) &= \beta \lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( \chi_n A \chi_n C^{Wick} B \right) \\ &= \beta \lim_{k \rightarrow \infty} \omega_{\varepsilon_k} \left( \chi_n^2 A C^{Wick} B \right). \end{aligned}$$

Knowing, by Lemma B.1, that the Wigner measure of the sequence  $\{W(g)\rho_\varepsilon\chi_n^2(N_\varepsilon)W(f)\}$  is given by

$$\left\{ \mu e^{\sqrt{2}i\Re\langle f+g, u \rangle} \chi_n^2(\|u\|^2) \right\},$$

one concludes by [3, Thm. 6.13],

$$\lim_{\varepsilon \rightarrow 0} \omega_\varepsilon \left( A_n \frac{\alpha_{i\varepsilon\beta}(B_m) - B_m}{i\varepsilon} \right) = \int_{\ell^2(G)} \chi_n^2(\|u\|^2) e^{\sqrt{2}i\Re\langle f+g, u \rangle} C(u) d\mu.$$

□

**Corollary 4.6.** *Any Wigner measure of the  $(\alpha_t, \varepsilon\beta)$ -KMS family of states  $\omega_\varepsilon$  satisfies for all  $f, g \in \ell^2(G)$ ,*

$$\beta \int_{\ell^2(G)} \{e^{i\Re\langle g, u \rangle}; h(u)\} e^{i\Re\langle f, u \rangle} d\mu = \int_{\ell^2(G)} \{e^{i\Re\langle g, u \rangle}; e^{i\Re\langle f, u \rangle}\} d\mu. \quad (4.16)$$

*Proof.* It is a consequence of Proposition 4.3, Proposition 4.5 and dominated convergence while taking  $n, m \rightarrow \infty$ . □

Thus, we come to the following conclusion.

*Proof of Theorem 4.2.* The phase-space  $\ell^2(G)$  is a  $d$ -euclidean space. Let  $F, G$  be two smooth functions in  $\mathcal{C}_0^\infty(\ell^2(G))$ . The inverse Fourier transform gives,

$$F(u) = \int_{\ell^2(G)} e^{i\Re\langle f, u \rangle} \hat{F}(f) \frac{dL(f)}{(2\pi)^{d/2}}, \quad \text{and} \quad G(u) = \int_{\ell^2(G)} e^{i\Re\langle g, u \rangle} \hat{G}(g) \frac{dL(g)}{(2\pi)^{d/2}},$$

where  $\hat{F}, \hat{G}$  denote the Fourier transforms of  $F$  and  $G$  respectively. Multiplying the equation (4.16) by  $\hat{F}(f)\hat{G}(g)$  and integrating with respect to the Lebesgue measure in the variables  $f$  and  $g$ , one obtains

$$\beta \int_{\ell^2(G)} \{G(u), h(u)\} F(u) d\mu = \int_{\ell^2(G)} \{G(u), F(u)\} d\mu.$$

This proves the classical KMS condition (4.8). □

## 5. CLASSICAL KMS CONDITION

In this section, we point out that the only probability measure satisfying the classical KMS condition is the Gibbs equilibrium measure. This is a known fact and we provide here a short proof only for reader's convenience. The argument used below is borrowed from the work of M. Aizenman, S. Goldstein, C. Gruber, J. Lebowitz and P.A. Martin [2].

**Proposition 5.1** (Gibbs measure). *Suppose that  $\mu$  is a Borel probability measure on  $\ell^2(G)$  satisfying the classical KMS condition (4.8). Then  $\mu$  is the Gibbs equilibrium measure, i.e.,*

$$\frac{d\mu}{dL} = \frac{e^{-\beta h(u)}}{z(\beta)}, \quad \text{and} \quad z(\beta) = \int_{\ell^2(G)} e^{-\beta h(u)} dL(u),$$

with  $h(\cdot)$  is the classical Hamiltonian of the Discrete Nonlinear Schrödinger equation given by (4.6) and  $dL$  is the Lebesgue measure on  $\ell^2(G)$ .

*Proof.* Consider the Borel probability measure  $\nu = e^{\beta h(u)} \mu$ , so that for any Borel set  $\mathcal{B}$ ,

$$\nu(\mathcal{B}) = \int_{\mathcal{B}} e^{\beta h(u)} d\mu.$$

Note that, for any  $F, G \in \mathcal{C}_0^\infty(\ell^2(G))$ , the Poisson bracket satisfies

$$\{F e^{-\beta h(u)}, G\} = \{F, G\} e^{-\beta h(u)} - \beta \{h, G\} F(u) e^{-\beta h(u)}.$$

Hence, the classical KMS condition (4.8) can be written as

$$\mu \left( e^{\beta h(u)} \{F e^{-\beta h(u)}, G\} \right) = 0,$$

or equivalently for any  $F, G \in \mathcal{C}_0^\infty(\ell^2(G))$ ,

$$\nu \left( \{F e^{-\beta h(u)}, G\} \right) = 0.$$

Remark that the classical Hamiltonian  $h$  is a smooth  $\mathcal{C}^\infty(\ell^2(G))$  function. Hence, the measure  $\nu$  satisfies for any  $F, G \in \mathcal{C}_0^\infty(\ell^2(G))$ ,

$$\nu \left( \{F, G\} \right) = 0.$$

This condition implies that  $\nu$  is a multiple of the Lebesgue measure. Indeed, take  $g(\cdot) = \langle e_j, \cdot \rangle \varphi(\cdot)$  with  $\varphi \in \mathcal{C}_0^\infty(\ell^2(G))$  being equal to 1 on the support of  $f$ . Then the Poisson bracket gives,

$$\{f, g\} = -i \partial_j f.$$

So, in a distributional sense the derivatives of the measure  $\nu$  are null and therefore  $d\nu = c dL$  for some constant  $c$ . Using the normalisation requirement for  $\mu$ , one concludes that  $d\nu = \frac{1}{z(\beta)} dL$ .  $\square$

## APPENDIX A. NUMBER ESTIMATES

Consider the quasi free state  $\omega_\varepsilon^0(\cdot)$  given by,

$$\omega_\varepsilon^0(\cdot) = \frac{\text{tr} \left( \cdot e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)} \right)}{\text{tr} \left( e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)} \right)}.$$

The following uniform number of particles estimates are well know. Here we recall them for reader's convenience. For more details on quasi free states and such inequalities, see e.g. [9, 21, 16]. Remember that the rescaled number operator is given by,

$$N_\varepsilon := \varepsilon d\Gamma(1_{\ell^2(G)}) = \varepsilon \sum_{x \in V} a_x^* a_x.$$

**Lemma A.1.** *For any  $k \in \mathbb{N}$ , there exists a positive constant  $c_k$  such that*

$$\omega_\varepsilon^0(N_\varepsilon^k) \leq c_k,$$

*uniformly with respect to  $\varepsilon \in (0, \bar{\varepsilon})$ .*

**Lemma A.2.** *There exists a positive constant  $c$  such that*

$$\frac{\text{tr}(e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)})}{\text{tr}(e^{-\beta H_\varepsilon})} \leq c,$$

*uniformly with respect to  $\varepsilon \in (0, \bar{\varepsilon})$ .*

*Proof.* By using a Bogoliubov type inequality, see [27, Appendix D], one has that

$$\ln(\operatorname{tr}(e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)})) - \ln(\operatorname{tr}(e^{-\beta H_\varepsilon})) \leq \beta \frac{\operatorname{tr}(\varepsilon^2 \frac{\lambda}{2} I_G e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)})}{\operatorname{tr}(e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)})}.$$

According to Definition 2.1, recall that

$$I_G = \sum_{x \in V} a_x^* a_x^* a_x a_x.$$

Therefore, there exists  $c > 0$  such that

$$\ln(\operatorname{tr}(e^{\beta \varepsilon d\Gamma(\Delta_G + \kappa 1)})) - \ln(\operatorname{tr}(e^{-\beta H_\varepsilon})) \leq c (\omega_\varepsilon^0(N_\varepsilon^2) + \omega_\varepsilon^0(N_\varepsilon)).$$

Using Lemma A.1, one proves the inequality.  $\square$

**Lemma A.3.** *For any  $k \in \mathbb{N}$ , there exists a positive constant  $c_k$  such that*

$$\omega_\varepsilon(N_\varepsilon^k) \leq c_k,$$

*uniformly with respect to  $\varepsilon \in (0, \bar{\varepsilon})$ .*

*Proof.* A direct consequence of Lemma A.1, Lemma A.2 and the Golden-Thompson inequality.  $\square$

## APPENDIX B. TECHNICAL ESTIMATES

We refer the reader to [3] for more details in the semiclassical analysis on the Fock space. Here, we only sketch some useful technical results based in the above work. Remember that the KMS states  $\omega_\varepsilon$ , given by (3.2), are normal and so we denote,

$$\omega_\varepsilon(\cdot) = \operatorname{tr}_{\mathfrak{F}}(\rho_\varepsilon \cdot).$$

Furthermore, assume for a subsequence  $(\varepsilon_k)_{k \in \mathbb{N}}$ , such that  $\lim_{k \rightarrow \infty} \varepsilon_k = 0$ , that the set  $\{\rho_{\varepsilon_k}\}_{k \in \mathbb{N}}$  admits a unique Wigner measure  $\mu$ . Then the following result holds true.

**Lemma B.1.** *For any  $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$  and  $f, g \in \ell^2(G)$ , the set  $\{W(f)\rho_{\varepsilon_k}\chi(N_{\varepsilon_k})W(g)\}_{k \in \mathbb{N}}$  admits a unique Wigner measure given by*

$$\{\mu e^{\sqrt{2}i\Re\langle f+g, u \rangle} \chi(\|u\|^2)\}.$$

*Proof.* For simplicity, we denote  $\varepsilon$  instead of  $\varepsilon_k$ . It is enough to prove that the set of Wigner measures for the density matrices  $\{\rho_\varepsilon \chi(N_\varepsilon)\}$  is the singleton

$$\{\mu \chi(\|u\|^2)\}.$$

In fact, using the Weyl commutation relations, one checks according to (4.5),

$$\lim_{\varepsilon \rightarrow 0} \operatorname{tr}_{\mathfrak{F}}(W(f)\rho_\varepsilon \chi(N_\varepsilon)W(g)W(\eta)) = \int_{\ell^2(G)} e^{i\sqrt{2}\Re\langle f+g+\eta, u \rangle} d\nu,$$

where  $\nu$  is a Wigner measure of the set of density matrices  $\{\rho_\varepsilon \chi(N_\varepsilon)\}$ . Now, using Pseudo-differential calculus,

$$\chi(N_\varepsilon) = (\chi(\|u\|^2))^{Weyl} + O(\varepsilon),$$

where the subscript refers to the Weyl  $\varepsilon$ -quantization and the difference between the right and left operators is of order  $\varepsilon$  in norm (see e.g. [12, Thm. 8.7]). Then [3, Thm. 6.13] with Lemma A.3, gives

$$\nu = \mu \chi(\|u\|^2).$$

$\square$

**Lemma B.2.** *For any  $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$  and  $f \in \ell^2(G)$ , there exists  $c > 0$  such that for all  $\varepsilon \in (0, \bar{\varepsilon})$ ,*

$$\|\chi(N_\varepsilon)[N_\varepsilon, W(f)]\chi(N_\varepsilon)\| \leq c\varepsilon, \quad \text{and} \quad \|\chi(N_\varepsilon)[H_\varepsilon, W(f)]\chi(N_\varepsilon)\| \leq c\varepsilon.$$

*Proof.* The proof of the two inequalities are similar. We sketch the second one. Using standard computation in the Fock space (see e.g. [3, Proposition 2.10]),

$$[H_\varepsilon, W(f)] = W(f) \left( h(\cdot + i\frac{\varepsilon}{\sqrt{2}}f) - h(\cdot) \right)^{Wick},$$

where the subscript refers to the *Wick* quantization, see [3, Section 2], and  $h$  is the classical Hamiltonian in (4.6). By Taylor expansion, one writes

$$h(u + i\frac{\varepsilon}{\sqrt{2}}f) - h(u) = \varepsilon C_\varepsilon(u),$$

where  $C_\varepsilon(u)$  is a polynomial in  $u$  which can be computed explicitly. Using the number estimate in [3, Lemma 2.5], one proves the inequality.  $\square$

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